

What is claimed is:

1. A method of analysing chemical data including a step of cluster analysis, the cluster analysis using a distance metric of the form:

$$D_{xy} = \frac{\sum_i \left(\left(\frac{x_i - c_i}{s_i} \right) - \left(\frac{y_i - c_i}{s_i} \right) \right)^2}{\sqrt{\left(\sum_i \left(\frac{x_i - c_i}{s_i} \right)^2 \right) \times \left(\sum_i \left(\frac{y_i - c_i}{s_i} \right)^2 \right)}}.$$

2. A method according to claim 1 that includes a step of performing principal component analysis on the data prior to the clustering step.
3. A method according to claim 1 that further includes a step of normalising the data prior to the clustering step.
4. A method according to claim 3 in which the normalising step modifies the data such that it has a mean value of 0 and a standard deviation of 1.
5. A method according to claim 1 that includes a further step of cluster analysis using a conventional distance metric.
6. A method according to claim 5 in which the further step of cluster analysis is applied to data that has not previously been assigned to a cluster.
7. A method according to claim 6 suitable for operation upon a set of data derived from the results of a chemical analysis programme.
8. A method according to claim 7 in which the analysis programme includes one or both of a quantitative structure-activity relationship (QSAR) analysis and a quantitative structure-property relationship (QSPR) analysis.

9. A method of analysing chemical data including a step of cluster analysis on 2-dimensional or 3-dimensional data, the cluster analysis using a distance metric for the distance between point x and point y of the form:

$$D(x,y) = 4\sin^2\left(\frac{\alpha}{2}\right) + \frac{(r_x - r_y)^2}{r_x r_y}, \text{ where } \alpha \text{ is the angle between point } x$$

5 and point y and r_x and r_y are, respectively, the distances from the co-ordinate origin to point x and point y .

10. A method according to claim 9 that includes a step of performing principal component analysis on the data prior to the clustering step.
11. A method according to claim 9 that further includes a step of normalising the
10 data prior to the clustering step.
12. A method according to claim 11 in which the normalising step modifies the data such that it has a mean value of 0 and a standard deviation of 1.
13. A method according to claim 9 that includes a further step of cluster analysis using a conventional distance metric.
- 15 14. A method according to claim 13 in which the further step of cluster analysis is applied to data that has not previously been assigned to a cluster.
15. A method according to claim 9 suitable for operation upon a set of data derived from the results of a chemical analysis programme.
- 20 16. A method according to claim 15 in which the analysis programme includes one or both of a quantitative structure-activity relationship (QSAR) analysis and a quantitative structure-property relationship (QSPR) analysis.
17. A computer program product for performing analysis of chemical data, the program being operative to perform a method including a step of cluster analysis, the cluster analysis using a distance metric of the form:

$$D_{xy} = \frac{\sum_i \left(\left(\frac{x_i - c_i}{s_i} \right) - \left(\frac{y_i - c_i}{s_i} \right) \right)^2}{\sqrt{\left(\sum_i \left(\frac{x_i - c_i}{s_i} \right)^2 \right) \times \left(\sum_i \left(\frac{y_i - c_i}{s_i} \right)^2 \right)}}.$$

18. A computer program product according to claim 17 that has as an input a set of machine-readable data representative of the results of a chemical analysis programme.
- 5 19. A computer program product according to claim 18 in which the analysis programme includes a quantitative structure-activity relationship (QSAR) analysis and a quantitative structure-property relationship (QSPR) analysis.
20. A computer program product for performing analysis of chemical data, the program being operative to perform a method including a step of cluster analysis on 2-dimensional or 3-dimensional data, the cluster analysis using a distance metric of the form:

$$D(x, y) = 4 \sin^2\left(\frac{\alpha}{2}\right) + \frac{(r_x - r_y)^2}{r_x \cdot r_y},$$

where α is the angle between point x and point y and r_x and r_y are, respectively, the distances from the co-ordinate origin to point x and point y .
- 10 21. A computer program product according to claim 20 that has as an input a set of machine-readable data representative of the results of a chemical analysis programme.
- 15 22. A computer program product according to claim 21 in which the analysis programme includes a quantitative structure-activity relationship (QSAR) analysis and a quantitative structure-property relationship (QSPR) analysis.
- 20